

Propane, 2-methyl-1-nitro-  
625-74-1 | DTXSID90211547

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 23.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.85e-01

Confidence level: 5.56e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Toluene</div> <div>Measured: 117</div> <div>Predicted: 87.4</div>	<div>Image not found</div> <div>Resorcinol</div> <div>Measured: 9.55</div> <div>Predicted: 28.3</div>	<div>Image not found</div> <div>Phenol</div> <div>Measured: 26.9</div> <div>Predicted: 57.3</div>
<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 3.16</div> <div>Predicted: 8.95</div>	<div>Image not found</div> <div>Butylamine</div> <div>Measured: 75.9</div> <div>Predicted: 19.9</div>	